

HPC workflow compartmentalise a multiscale simulation aimed at the personalisation of COVID-19 treatments and facilitate its scalability

Vincent Noël^{1,*}, Javier Conejero^{2,*}, Jose Carbonell², Miguel Vázquez², Gaurav Saxena², Miguel Ponce de Leon², Thalia Diniaco², David Vicente², Emmanuel Barillot¹, Laurence Calzone¹, Rosa M Badia², Alfonso Valencia^{2,3,\$} and Arnau Montagud^{2,\$}

1 Institut Curie, INSERM U900, Mines ParisTech, University PSL, Paris, France

2 Barcelona Supercomputing Center, Barcelona, Spain

3 Institució Catalana de Recerca i Estudis Avançats (ICREA), Barcelona, Spain

(*) co-first authors

(\$) co-last authors

Information on the tools and projects:

- PerMedCoE

Website: <http://permedcoe.eu/>; Twitter: <https://twitter.com/PerMedCoE/>

- PerMedCoE COVID-19 multiscale modelling workflow

Code repository: <https://github.com/PerMedCoE/PilotWorkflow>

- PhysiCell

Ghaffarizadeh A, et al. PhysiCell: An open source physics-based cell simulator for 3-D multicellular systems. PLOS Comput Biol. 2018;14:e1005991.

Code repository: <https://github.com/MathCancer/PhysiCell>

- PhysiCell 4 COVID initiative

Getz M, et al. Rapid community-driven development of a SARS-CoV-2 tissue simulator. bioRxiv. 2020;2020.04.02.019075.

Code repository: <https://github.com/pc4covid19/COVID19>;
<https://zenodo.org/record/3954019>

- MaBoSS

Stoll G, et al. MaBoSS 2.0: an environment for stochastic Boolean modeling. Bioinformatics. 2017;33:2226–8.

Code repository: <https://github.com/maboss-bkmc/MaBoSS-env-2.0>

- PhysiBoSS

Letort G, et al. PhysiBoSS: a multi-scale agent-based modelling framework integrating physical dimension and cell signalling. Bioinformatics. 2019;btz766.

Code repository: <https://github.com/bsc-life/PhysiBoSSv2>

PhysiBoSS-COVID code repository: <https://github.com/vincent-noel/COVID19>

- COVID-19 Disease Map (C19DM) initiative

Ostaszewski, M. et al. COVID19 Disease Map, a computational knowledge repository of virus–host interaction mechanisms. Molecular Systems Biology. 2021; 17, e10387.

Website: <http://doi.org/10.17881/covid19-disease-map>; <https://git-r3lab.uni.lu/covid/models>

- BioFVM-X

Saxena G, et al. BioFVM-X: An MPI+OpenMP 3-D Simulator for Biological Systems in Computational Methods in Systems Biology (eds. Cinquemani, E. & Paulevé, L.).2021; 266–279

Code repository: https://gitlab.bsc.es/g saxena/biofvm_x

- PyCOMPSs

Tejedor E, et al. PyCOMPSs: Parallel computational workflows in Python. The International Journal of High Performance Computing Applications. 2017; 31(1), 66–82.

Code repository: <https://github.com/bsc-wdc/compss>

- Singularity containers

Kurtzer GM, et al. Singularity: Scientific containers for mobility of compute. PLoS ONE. 2017; 12(5): e0177459

Website: <https://apptainer.org/>; <https://github.com/apptainer/apptainer>